Discovery and Optimization of Novel High Performance Polyolefin Catalysts

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Introduction

Symyx Technologies is a leading company for high productivity R&D. [1] We are active in the area of both homogeneous and heterogeneous catalysis and have established a high throughput platform for polymerization catalysis research and development. [2,3] Multiple catalyst families have been discovered and optimized for their performance.

Materials and Methods

We use an integrated approach to discover hits and optimize catalyst candidates for the polymerization of olefins in homogeneous and slurry phase. The following methods are employed:

- "Workflows" resemble assembly lines, allowing methodical and efficient generation of arrays ("Libraries") of new classes of materials
- "Library" format designed to maximize the ease of screening for various catalytic and material properties
- High-speed robotic catalyst synthesis and testing technologies
- Rapid analytical tools to characterize polymeric structure
- Rapid polymer property testing tools to directly measure key mechanical and processing properties, enabling property-driven materials discovery
- Iterative loops of optimization

Results and Discussion

We will discuss the evolution of multiple new catalyst families from their first discovery over iterative loops of optimization to achieve commercially viable catalysts systems. Case studies will be presented to illustrate the Symyx high productivity research platforms.

References

1. **http://www.symyx.com/research/catalysis**
2. Boussie et al., *JACS*, **2003**, 125(14), pp4306-4317
3. Boussie *et al., Angew. Chem. Int. Ed.* **2006**, *45*, pp3278-3283.